FISSION NUMERICS ERRORS AND CORRECTIONS*

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Possible errors in calculations of T_{sf} of atomic nuclei are discussed. The methods of improving the results are briefly presented.

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1. Introduction

The theoretical works in fission focus mainly on determination of some important parameters characteristic for fission of different nuclei. These are potential energy barriers (height, stiffness, locations of minima and maxima), mass parameters and spontaneous fission half lives T_{sf} [1]. In most cases one examines only the fission from the ground state of mother nucleus into the ground states of two identical fission fragments. There hardly exist models which describe the more complicated situations.

Analytical complexity of the problem does not allow for closed formulae and the results in fission research are usually numerical. It is notable that almost all calculations of spontaneous fission half lives T_{sf} have been performed in the framework of conventional Wentzel-Kramers-Brillouin (WKB) approximation.

The experienced computer users know that *the numerical results depend on the number of operations.* It is a practical result of computations. It seems odd only on the first sight. There are usually two reasons of cumulating errors in computations. *i)* model approximations and *ii)* improper numerical methods used to solve a given theoretical problem. The first source of errors, which we call generic, is very important. However, in the

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present paper we deal mainly with numerical methods. In the present paper we study the dependence of spontaneous fission half lives T_{sf} on some common numerical techniques used in fission calculations.

2. Model calculations of half lives T_{sf}

As the basis for the calculation of energy and mass parameters of fissioning nuclei we took the Nilsson single particle model hamiltonian. The deformation space of the nucleus is reduced to one degree of freedom ε which describes the elongation of the nuclear shape. The reduction to lowest dimension produces major technical simplifications while maintaining enough of the flavour of the more dimensional case to produce valuable insight into the full model. To make the model realistic we include the *pairing* forces in the BCS approximation and we take standard Strutinsky model of the nuclear energy.

The inertia of the nucleus against elongation is the second rank tensor in one dimensional deformation space. In the following we use the *cranking* approximation of it.

3. Tunnelling

In the classical WKB approximation the probability of tunnelling reads

$$P = (1 + \mathrm{e}^{S})^{-1}, \tag{1}$$

where the action ($\hbar$ units) reads

$$S = 2 \int_{\varepsilon_1}^{\varepsilon_2} \sqrt{2[V(\varepsilon) - E_{\mathrm{fiss}}]\, B(\varepsilon)}\, ds. \tag{2}$$

The half life time T_{sf} is inversely proportional to the tunnelling probability

$$T_{sf} = \frac{\ln 2}{nP}. \tag{3}$$

Here n is the number of assaults of the nucleus on the fission barrier in the time unit. Taking for zero point energy the value 0.5 MeV one finds $n = \omega/(2\pi) = \hbar\omega/(\pi\hbar) = 0.5\ \mathrm{MeV}\, c/(\pi c\hbar) \approx 10^{20.38}/s$. Here c is the vacuum velocity of light. It should be emphasized that taking a constant value of $\hbar\omega$ leads to the kind of averaging of the dynamical ground state properties of nuclei. The oscillator model of nuclear vibrational motion gives $\hbar\omega = \sqrt{C(\varepsilon_{\mathrm{eq}})/B(\varepsilon_{\mathrm{eq}})}$, where $C(\varepsilon_{\mathrm{eq}}) = \left(d^2V/d\varepsilon^2\right)_{\mathrm{eq}}$ and the subscript

"eq" means the deformation at minimum of the potential energy. This shows that the assumption of a constant $\hbar\omega$ is a very weak assumption of the model. It is the generic error of the fission model. Conclusion: *The value of this parameter should be calculated for each nucleus separately.*

4. Results

The calculations are performed in the simple one dimensional model. We consider the group of even-even Fermium isotopes convenient for our studies, since it is believed that the standard results of calculations of T_{sf} for these isotopes reproduce experimental data with a very good accuracy.

The density of grid points (in which potential and inertia are calculated) is decisive for accuracy of approximations and influences strongly the final results. We shall prove this statement.

The energy $V(\varepsilon)$ and the mass $B(\varepsilon)$ were (typically) calculated at deformation points with distance $\Delta\varepsilon = 0.05$ between them. We have done the calculations in four independent cases in which calculation points were shifted to the right on the distance $\delta = 1/4\Delta\varepsilon = 0.0125$. Results for energy nearly coincide for all cases.

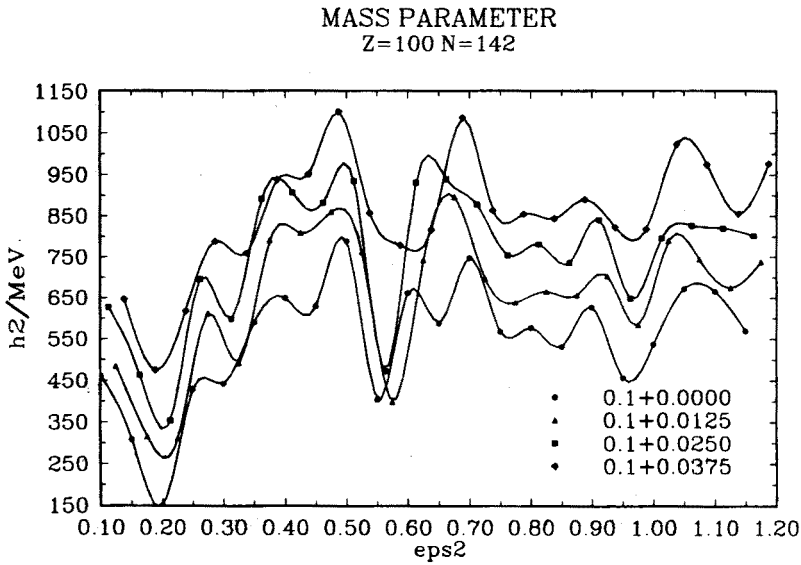

Fig. 1. The mass parameter of the isotope ^{242}Fm for four cases of deformation lattice. The successive curves show the results as obtained for lattices shifted with respect to the basic lattice (lower case) by 0.0125, 0.0250 and 0.0375. For clarity, all curves are shifted by $100\hbar^2$ MeV^{-2}.

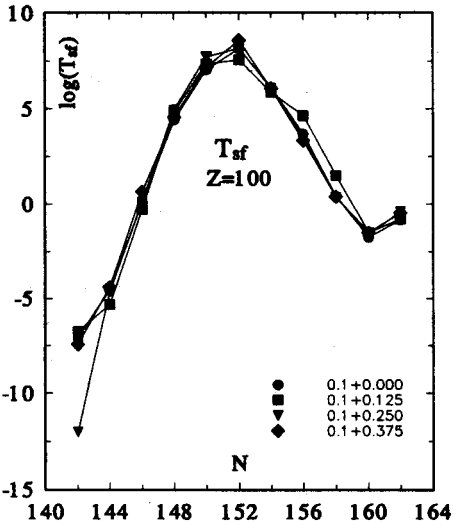

Fig. 2. The logarithms of spontaneous fission half lives T_{sf} of Fermium isotopes. The successive curves show the results as obtained for lattices shifted with respect to the basic lattice (lower case) by 0 (•), 0.0125 (■), 0.0250 ($\bigtriangledown$) and 0.0375($\diamond$).

In Fig. 1, we show the mass parameter $B(\varepsilon)$ of the nucleus ^{242}Fm. The differences between the considered cases of different deformation lattices are large and range from 20 to 30% of B. The logarithms of corresponding half lives T_{sf} (years) are shown in Fig. 2. The range of $\log T_{sf}$ changes from 0.5 to 3.5 orders of magnitude. So the large errors are incorporated through the choice of calculation points.

These divergences can be obtained from the variation of the formula (3). Discarding 1 in comparison to e^S, and taking relative errors $\delta V/V \approx 0$ and $\delta B/B \approx 0.3$ (see above) one obtains

$$\frac{\delta T_{sf}}{T_{sf}} = 0.15S. \tag{4}$$

For nuclei considered here S is of the order of 10. The relative change of T_{sf} is then of the order of 1 (see Fig. 2).

The second numerical test gives the dependence of errors on the distance between the lattice points. We made the series of five different numerical runs. Each calculation was performed for different lattice links: $\Delta\varepsilon = 0.1, 0.05, 0.025, 0.02, 0.01$. The functional dependence of mass parameters on deformation stabilizes at grid points density corresponding to the lattice link distance $\Delta\varepsilon < 0.025$.

The results of T_{sf} calculations for all Fermium isotopes are displayed in Fig. 4. The logarithms of T_{sf} are shown here as vertical bars. Assuming

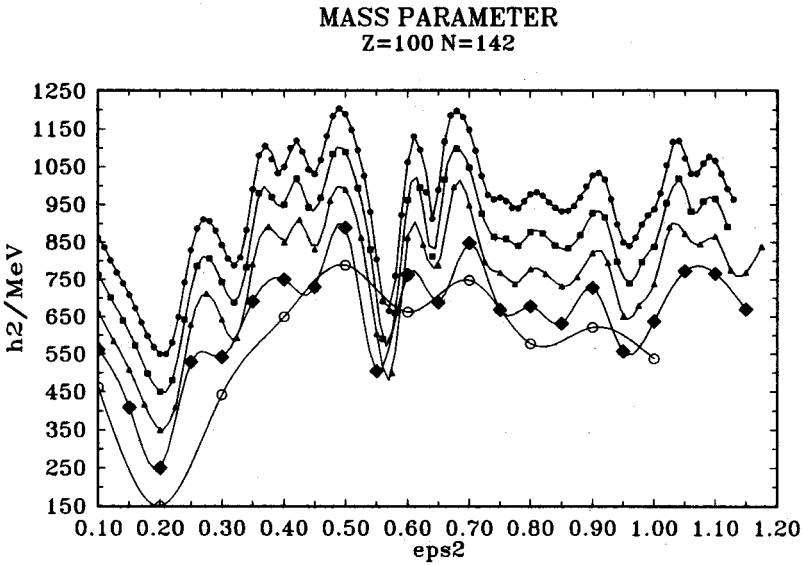

Fig. 3. The mass parameter $B(\varepsilon)$ of the isotope ^{242}Fm in five cases of deformation lattice. The results are for the following densities of the grid points: $\Delta\varepsilon = 0.1$, 0.05, 0.025, 0.02, 0.01. For clarity, the curves are shifted by 100 mass parameter units.

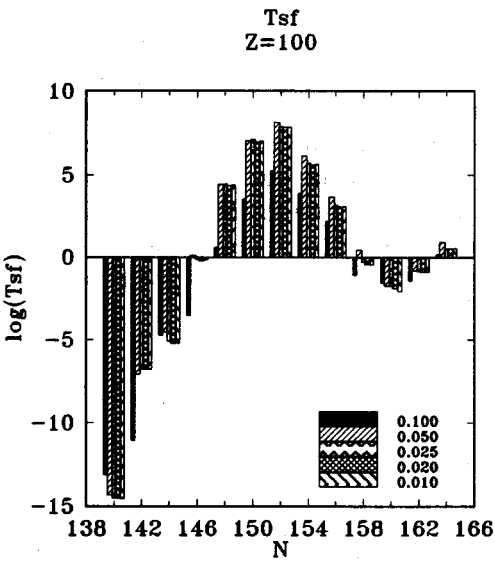

Fig. 4. The logarithms of spontaneous fission half lives T_{sf} of Fermium isotopes. The following lattice densities are displayed: $\Delta\varepsilon = 0.1$, 0.05, 0.025, 0.02, 0.01.

for the moment that the T_{sf} values calculated for the density $\Delta\varepsilon = 0.01$ are practically exact we see the following:

- Choosing the deformation lattice link $\Delta\varepsilon = 0.1$ we make an error in T_{sf} calculations reaching three orders of magnitude.
- The lattice with the link length $\Delta\varepsilon = 0.05$ produces an error in T_{sf} ranging from 0.5 to 1.5 orders of magnitude.
- A numerical error smaller than 0.5 can be obtained only in the case of $\Delta\varepsilon \leq 0.025$. It should be remembered that the whole calculation presented above was done for one degree of freedom. All the errors can augment in a more dimensional case.

The calculations can be improved if the computations of fission barrier and mass parameter are done at gaussian points. One needs to find the entrance and the exit points for a given fission barrier. They are distinct for different nuclei (different zero point energy). We see that we have to calculate twice the potential energy of the system (it is approximately equivalent to the "normal" calculations for the all considered nuclei): *i)* determine exit/entrance points and *ii)* calculate potential and mass parameters at gaussian points. Usually one takes into account 100 nuclei. This means hundreds of hours of work of the modern computers! Thus, the best receipt does not work here because of practical reasons.

5. Other errors

Except the errors mentioned above, there are still some interpretational errors. What are the half lives T_{sf} calculated in the assumed model of fission? Which "experimental" data should be compared to theoretical results? Here we point out one of possible dangers connected to this.

In experiment, one measures so called decay probabilities λ. These are the total probabilities of fission into all possible fission channels. The number of decays into the f^{th} channel is connected to the fission yield Y_f. In the case of a decay into n different channels one has $\lambda = \lambda_1 + \ldots + \lambda_n$. The total activity $\mathcal{A}$ is:

$$\mathcal{A} = -\frac{dN}{dt} = \lambda N_0 \exp(-\lambda t) = \mathcal{A}_0 \exp(-\lambda t). \tag{5}$$

The activity of decay in the k^{th} channel reads:

$$\mathcal{A}_k = -\frac{dN_k}{dt} = \lambda_k N = \lambda_k N_0 \exp(-\lambda t). \tag{6}$$

Since the yield Y_k is:

$$Y_k = \frac{\mathcal{A}_k}{\mathcal{A}} = \frac{\lambda_k}{\lambda}, \tag{7}$$

then the half life time $T_k^{\exp}$, corresponding to the decay in the k^{th} channel is:

$$T_k^{\exp} = \frac{1}{\lambda_k} = \frac{1}{\lambda Y_k}. \tag{8}$$

The theory gives the results for the one channel only. It follows that one has to compare T_{sf} to experimental half life times given by equation (8). According to our knowledge, this comparison has been done to the average half life time.

6. Summary

We have shown in a very simple fashion that the numerical calculations of spontaneous fission half lives performed very carefully may be contaminated with unexpected errors of both generic (model dependent) and numerical errors. There are also other errors which come from possibly wrong interpretation of T_{sf}.

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